Friedel Oscillation about a Friedel-Anderson Impurity

Yaqi Tao and Gerd Bergmann
Department of Physics & Astronomy
University of Southern California
Los Angeles, California 90089-0484
e-mail: bergmann@usc.edu

October 17, 2011

Abstract

The Friedel oscillations in the vicinity of a Friedel-Anderson (FA) impurity are investigated numerically. For an FA impurity in the local moment limit the normalized amplitude $A(\xi)$ is S-shaped, approximately zero at short distances, approaching two at large distances and crossing the value one at the characteristic length $\xi_{1/2}$. Surprisingly, the Friedel oscillations of a simple non-interacting Friedel impurity with a narrow resonance at the Fermi level show a very similar behavior of their amplitude $A(\xi)$. A comparison correlates the resonance width and the Kondo energy of the FA impurity with the characteristic length $\xi_{1/2}$ of the Friedel oscillations.

PACS: 75.20.Hr, 71.23.An, 71.27.+a , 05.30.-d

1 Introduction

The properties of magnetic impurities in a metallic host were first studied theoretically by Friedel [1] and Anderson [2]. Kondo [3] showed that a magnetic impurity with spin-flip scattering develops a singular behavior at low temperatures. As a consequence the ground state is a singlet state with zero effective magnetic moment. Schrieffer and Wolff [4] showed that the Friedel-Anderson (FA) Hamiltonian can be transformed into a Kondo Hamiltonian plus a number of additional terms. Its ground state is also a singlet state. The disappearance of the magnetic moment at low temperatures, the Kondo effect, is one of the most intensively studied problems in solid state physics , [5], [6], [7], [8], [9], [10], [11], [12], [13], [14], [15], [16], [17], [18], [19]. In the last decade the Kondo effect has experienced a renaissance. There is a growing interest in this field [20], extending from magnetic atoms on the surface of corrals [21] to carbon nanotubes [22], quantum dots [23], [24], [25], [26], [27], [28], [29] and nanostructures [30]. There are still many open questions, particularly the real-space form of the wave function and the resulting charge density and polarization.

Affleck, Borda and Saleur [31] (ABS) investigated the formation of Friedel oscillations in the vicinity of a Kondo impurity. The oscillating part of the electron charge has the following form.

$$\rho_{Fr}(r) = \frac{C_D}{r^D}\left[A(r)\cos\left(2k_F r + D\frac{\pi}{2}\right)\right] \tag{1}$$

where D is the dimension of the system, the coefficients C_D have the values $C_1 = 1/(2\pi)$, $C_2 = 1/(2\pi^2)$ and $C_3 = 1/(4\pi^2)$. They succeeded in calculating the asymptotic form of the function $A(r)$ (which is a universal funtion of r/r_K, $r_K = \hbar v_F/(k_B T_K)$= Kondo length) from first principles and performed a numerical calculation using NRG (numerical renormalization group). $A(r)$ approaches the values two for $r >> r_K$ and zero for $r << r_K$. One of the authors [32] applied the approximate solution of the FAIR theory (Friedel Artificially Inserted Resonance) to reproduce the result by ABS. The two calculations confirm each other.

In the same paper one of the authors showed that a simple non-interacting Friedel impurity with its resonance at the Fermi energy showed Friedel oscillations similar to the Kondo impurity. This reveals the interesting fact that the complex interacting Kondo impurity yields Friedel oscillations very similar to those of a simple resonance of a non-interacting electron gas. In both cases the amplitude $A(r)$ approaches zero for $r << r_R$ and for $r >> r_R$ each spin contributes the value one to the amplitude. The transition happens at a characteristic length which is of the order of $r_R = \hbar v_F/\Gamma$ with v_F being the Fermi velocity and Γ the half-width of the resonance.

It had been observed earlier that the Friedel phase shifts and sum rules that were derived for non–interacting electron systems also apply to interacting electron systems (see for example [**?**]). This can be a great help in describing interacting electron systems, which are generally not very transparent. A very good example is the Kondo impurity with its Kondo resonance [**?**], [**?**], [**?**], [21]. However, the opinion of experts (in private conversations) are extremely divided, ranging from "there is really no Kondo resonance" to " yes there is a Kondo resonance but its form is very complicated and nobody can write it down". Therefore it is a considerable help when the complex system follows the same simple rules as a single electron system. In this paper we calculate the Friedel oscillations of the Friedel-Anderson (FA) impurity and demonstrate their similarity with the Friedel oscillations of a simple non-interacting Friedel impurity.

2 Theoretical Background

The FA Hamiltonian consists of spin-up and down free electron states $c_{\nu,\sigma}^{\dagger}$, a d-resonance $d_{\sigma}^{\dagger}$ with the energy E_d and s-d-hopping matrix elements V_{ν}^{sd} between the conduction electrons and the d-impurity. A simultaneous occupation $n_{d\uparrow}$ and $n_{d\downarrow}$ of the d-resonance contributes a Coulomb exchange energy $Un_{d\uparrow}n_{d\downarrow}$.

$$H_{FA} = \sum\nolimits_{\sigma}\left\{\sum_{\nu=0}^{N-1}\varepsilon_{\nu}c_{\nu\sigma}^{\dagger}c_{\nu\sigma} + \sum_{\nu=0}^{N-1}V_{\nu}^{sd}[d_{\sigma}^{\dagger}c_{\nu\sigma} + c_{\nu\sigma}^{\dagger}d_{\sigma}] + E_d d_{\sigma}^{\dagger}d_{\sigma}\right\} + Un_{d\uparrow}n_{d\downarrow} \tag{2}$$

The FA impurity shows also the Kondo effect as Schrieffer and Wolff [4] have shown. The FA impurity has many degrees of freedom. Its behavior is determined by the d-resonance energy E_d, the Coulomb energy U and the s-d-scattering matrix element $|V_{sd}|^2$. For simplicity we will discuss here the symmetric FA impurity with $E_d = -U/2$.

For sufficiently large values of $U/|V_{sd}|^2$ the FA impurity possesses a magnetic moment above the Kondo temperature. One difficulty in determining the magnetic moment is the fact that the magnetic state is not the ground state of the system. The ground state is a singlet state (or Kondo state) with vanishing the total moment, whose energy is lowered by the Kondo energy. For many realistic systems the Kondo energy is quite small. If warmed above the Kondo temperature the FA impurity is magnetic, but it is still at rather low temperature. We denote this as the magnetic pseudo-ground state. In the FAIR approach the magnetic wave function has the form

$$\Psi_{MS} = \left[A a_{0\uparrow}^{\dagger} b_{0\downarrow}^{\dagger} + B a_{0\uparrow}^{\dagger} d_{\downarrow}^{\dagger} + C d_{\uparrow}^{\dagger} b_{0\downarrow}^{\dagger} + D d_{\uparrow}^{\dagger} d_{\downarrow}^{\dagger} \right] \prod_{i=1}^{n-1} a_{i\uparrow}^{\dagger} \prod_{i=1}^{n-1} b_{i\downarrow}^{\dagger} \Phi_0 \tag{3}$$

Here $a_{0\uparrow}^{\dagger}$ and $b_{0\downarrow}^{\dagger}$ are two artificially inserted Friedel resonances with a composition

$$a_{0\uparrow}^{\dagger} = \sum_{\nu} \alpha_0^{\nu} c_{\nu\uparrow}^{\dagger}$$

(As discussed in previous papers [33] the FAIR states have a relatively simple interpretation in Hilbert space.) The remaining states in the spin up basis are $\left\{ a_{i\uparrow}^{\dagger} \right\}$ which are orthogonal to each other and to $a_{0\uparrow}^{\dagger}$.In addition the free electron Hamiltonian $H_{0\uparrow}$ for spin-up electrons is made sub-diagonal in this basis, i.e. all matrix elements $\left\langle a_{\nu\uparrow}^{\dagger} \left| H_{0\uparrow} \right| a_{\mu\uparrow}^{\dagger} \right\rangle = \delta_{\nu,\mu}$ for $\nu, \mu \neq 0$. As a consequence the whole basis is fully determined by $a_{0\uparrow}^{\dagger}$. The FAIR state $b_{0\downarrow}^{\dagger}$ with its basis $\left\{ b_{i\downarrow}^{\dagger} \right\}$ has analogous properties. The details of the FAIR theory are described in previous papers [34], [35], [36], etc.

The mean field theory produces two d-resonances in the magnetic state, one for the spin-up band at $E_d + Un_{d\downarrow}$ and another one for the spin-down band at $E_d + Un_{d\uparrow}$. Here $n_{d\uparrow}, n_{d\downarrow}$ are the partial occupations of the spin-up and -down d-resonances. In mean field theory these resonances have the half width $\Gamma = \pi |V_{sd}|^2 \rho$ (ρ=density of states). Mean field theory completely decouples the s-d-scattering between different spin bands. In reality a doubly occupied d-state decays in both spin bands, and the decay rate is twice as large [37]. The FAIR theory of the magnetic state yields d-resonances with the correct resonance width [38].

The ground state of the FA impurity is a singlet state. The latter is obtained in FAIR by reversing all spins in equ. (3). After ordering the spin sequences the two states are added and normalized. For the singlet state the composition of the FAIR states $a_0^{\dagger}$ and $b_0^{\dagger}$ has to be optimized again (and is very different from the composition in the magnetic state). The two (opposite) magnetic states in (4) are not orthogonal to each other and yield a finite interference between the two magnetic components. The strength of this interference determines the Kondo energy.

$$\Psi_{SS} = \tag{4}$$
$$\left\{\begin{array}{ll} & \left[Aa_{0\uparrow}^{\dagger}b_{0\downarrow}^{\dagger}+Ba_{0\uparrow}^{\dagger}d_{\downarrow}^{\dagger}+Cd_{\uparrow}^{\dagger}b_{0\downarrow}^{\dagger}+Dd_{\uparrow}^{\dagger}d_{\downarrow}^{\dagger}\right]\prod_{i=1}^{n-1}a_{i\uparrow}^{\dagger}\prod_{i=1}^{n-1}b_{i\downarrow}^{\dagger}\Phi_0 \\ + & \left[A'b_{0\uparrow}^{\dagger}a_{0\downarrow}^{\dagger}+B'd_{\uparrow}^{\dagger}a_{0\downarrow}^{\dagger}+C'b_{0\uparrow}^{\dagger}d_{\downarrow}^{\dagger}+D'd_{\uparrow}^{\dagger}d_{\downarrow}^{\dagger}\right]\prod_{i=1}^{n-1}b_{i\uparrow}^{\dagger}\prod_{i=1}^{n-1}a_{i\downarrow}^{\dagger}\Phi_0 \end{array}\right\}$$

In the numerical calculation we use the Wilson band [12] which is an electron-hole symmetric band, normalized by the Fermi energy and extending from $(-1<\varepsilon<+1)$ with a constant density of states $\rho=1/2$. The electron states in the Wilson band are represented by a finite number of Wilson states. We generally start our numerical calculation with $N=60$ Wilson states with energies of $\pm\frac{3}{4},\pm\frac{3}{8},\pm\frac{3}{16},..\ \pm\frac{3}{2^{30}},\pm\frac{1}{2^{30}}$. The ratio between neighboring energies is $\Lambda=2$ (except for the two states next to the Fermi level). The wave function of the Wilson states in real space is described in previous papers [39], [32]. From the composition of the two bases $\left\{a_i^{\dagger}\right\}$ and $\left\{b_i^{\dagger}\right\}$ in terms of the Wilson states $c_{\nu}^{\dagger}$ one obtains their wave functions in real space.

The calculation in real space can be done in one, two or three dimensions. The results differ by the dimensional factor $C_D/r^D$and the phase shift $-D\frac{\pi}{2}$ (see equ.(1)). If one splits off the dimensional factor then we expect that the amplitude $A(r)$ is the same for all dimensions. Therefore we choose the simplest case, the one-dimensional FA impurity.

The calculation of the real space density at the position r is in principle straight forward but rather tedious due to the interference terms between the different bases. Here one has to calculate a large number of multi-electron scalar products in form of determinants. Fortunately this has to be done only once and can be used for all distances.

3 Numerical Results and Discussion

We performed the calculation of the Friedel oscillation for different combinations of parameters. In a first series we used for the s-d-hopping matrix element the value $|V_{sd}|^2=0.03$ and for the Coulomb energy the values $U=0.1$, 0.2, 0.4, 0.6, 0.8 and 1.0 with $E_d=-U/2$. In the first round 60 Wilson states with energies of $\pm\frac{3}{4},\pm\frac{3}{8},\pm\frac{3}{16},..\ \pm\frac{3}{2^{30}},\frac{1}{2^{30}}$ represented the free electron basis. As ABS already noticed the Wilson states with an energy ratio of $\Lambda=2$ are so far apart in their energy that the results are not yet very accurate. (For example the Wilson state with the energy $\frac{3}{4}$ is composed of all states in the energy range of $\frac{1}{2}<\varepsilon<1$.This means that it has roughly an energy uncertainty of $\frac{1}{4}$. In simple words, the energy uncertainty of the Wilson states divided by the energy $\Delta E_W/E_W$ is about 1/3 for $\Lambda=2$). In the FAIR approach it is relatively easy to sub-divide the Wilson states geometrically [32]. The FAIR states $a_0^{\dagger}$ and $b_0^{\dagger}$ can be well interpolated during this procedure. From the FAIR states one obtains the whole bases $\left\{a_i^{\dagger}\right\}$ and $\left\{b_i^{\dagger}\right\}$.

After the first sub-division we have a new Wilson basis of 120 states with an energy ratio of $\Lambda=2^{1/2}$. The second sub-division yields 240 states with $\Lambda=2^{1/4}\approx 1.19$. Now even the

large energy levels lie close together, and the energy uncertainty $\Delta E_W/E_W$ takes the value of about 0.09.

In the calculation we measure the distance from the impurity in units of half the Fermi wave length λ_F, i.e. $\xi = 2r/\lambda_F$. In these units the Friedel oscillations have the period "one". We multiply the actually calculated amplitude by the factor $2\pi\xi$ to cancel the one-dimensional prefactor in equ. (1). The resulting normalized amplitude $A(\xi)$ is then valid for all dimensions of the sample.

In Fig.1 the Friedel oscillation amplitude $A(\xi)$ is shown as the function of the logarithm of the distance $\ell = \log_2(\xi)$ for the different parameters.

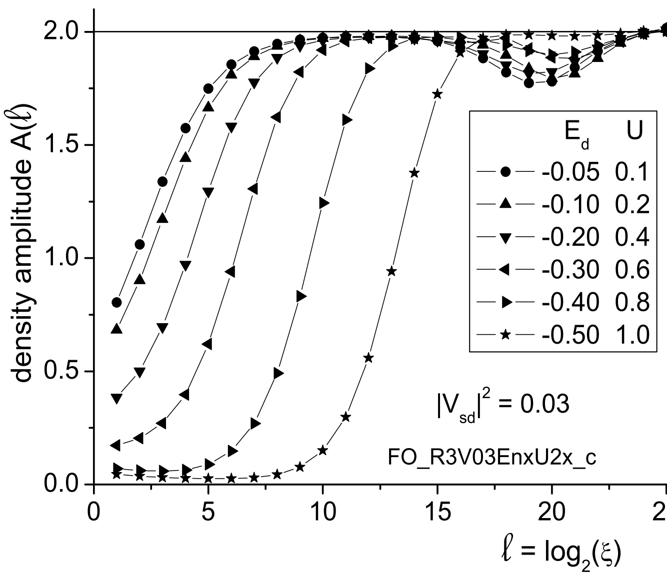

Fig.1: The amplitude $A(\ell)$ of the Friedel oscillations for a symmetric FA impurity with $|V_{sd}|^2 = 0.03$ and different values of U with $E_d = -U/2$. The abscissa is the distance $\ell = \log_2(\xi)$ from the impurity where $\xi = 2r/\lambda_F$.

The right curve (stars) in Fig.1 has the largest $U = 1$ and behaves very similar to a Kondo impurity that is discussed in ref. [31], [32]. For large distances the amplitude $A(\xi)$ reaches the value 2, and for short distances the amplitude essentially vanishes. The transition between these two regions occurs at the $\ell_{1/2}$-point where $A(\ell) = 1$. For $U = 0.8$ one obtains a similar curve as for $U = 1.0$, only shifted to the left. With decreasing U the $\ell_{1/2}$-point for the amplitude moves to shorter distances

For $U = 1$ and $U = 0.8$ the positions of the $\ell_{1/2}$-points are at 9.4 and 13.1. If one shifts one of the curves by 3.7 then one obtains a single curve. It represents the universal curve for the FA impurity with a full magnetic moment. If U is further decreased then the curves for $A(\xi)$ are further shifted to the left and for $U \leq 0.4$ they don't reach the horizontal axis anymore. Essentially the whole environment of the impurity is filled with Friedel oscillations.

Surprisingly the curves develop a small minimum at about $\ell = 20$ with decreasing value of U .

For the smallest value of $U = 0.1$ one is in the perturbative region while for $U = 1.0$ one is in the local moment region (see for example Krishna-murtha et al. [40]). Generally the properties of the symmetric FA impurity are characterized by the parameter $U/(\pi\Gamma) = U/\left(\pi^2 |V_{sd}|^2 \rho\right)$. In table I the values of $U/(\pi\Gamma)$ are collected for the different examples. Our curves for the Friedel oscillations approach the local moment behavior somewhere above $U/(\pi\Gamma) \approx 4$.

U	$\lvert V_{sd}\rvert^2$	**U/$\pi\Gamma$**	**r**	**S**
0.1	0.03	0.66	0.51	0.303
0.2	0.03	1. 33	0.67	0.354
0.4	0.03	2. 67	0.83	0.434
0.6	0.03	4.05	0.90	0.479
0.8	0.03	5. 33	0.93	0.497
1.0	0.03	6. 67	0.95	0.500

Table I: The effective coupling strength $U/(\pi\Gamma)$ for the different parameter of Fig.1. r and S are discussed in the text.

3.1 The magnetic half of the singlet state

The FAIR solution for the FA-impurity consists of two entangled magnetic states as shown in equ. (4). Each half in equ. (4) possesses a magnetic moment. For large $U/(\pi\Gamma)$ the magnetic moment is relatively well defined because the sum $S = (A^2 + B^2 + C^2 + D^2)$ is close to 0.5 and almost normalized to 1/2. If we define $r = (B^2 - C^2) / (A^2 + B^2 + C^2 + D^2)$ then the moment has the value $\mu/\mu_B \approx r$ as long as $S \approx 0.5$. However, with decreasing $U/(\pi\Gamma)$ the sum S becomes considerably smaller than 1/2 because it is the singlet state that is normalized, and the interference between the two magnetic parts becomes more and more important. The values of r and S are also collected in table I. It should, however, be emphasized that the magnetic moment of the magnetic half in the singlet state is not the same as the magnetic moment of the corresponding magnetic state as presented by equ. (3). Although the structure of the states is the same, the FAIR states $a_0^\dagger$ and $b_0^\dagger$ assume rather different composition.

For $U = 1, E_d = -0.5$ and $|V_{sd}|^2 = 0.03$ the magnetic halves of the singlet state are very well normalized to the value of $S = 0.500$. Therefore it is interesting to study their properties. In Fig.2 the half of the ground state with the net d-spin down is investigated. Both the spin-up and the spin-down bands of the conduction electron gas show charge oscillations with the period one. Their magnitudes are identical within the accuracy of the calculation. At large distances they reach the value $A = 0.5$. This means that the total charge oscillation of both spins for both magnetic components yields the value two which agrees with the results of Fig.1. However, for short distances one observes for each spin band a value of 0.05. This value appears to contradict the vanishing Friedel oscillations in Fig.1.

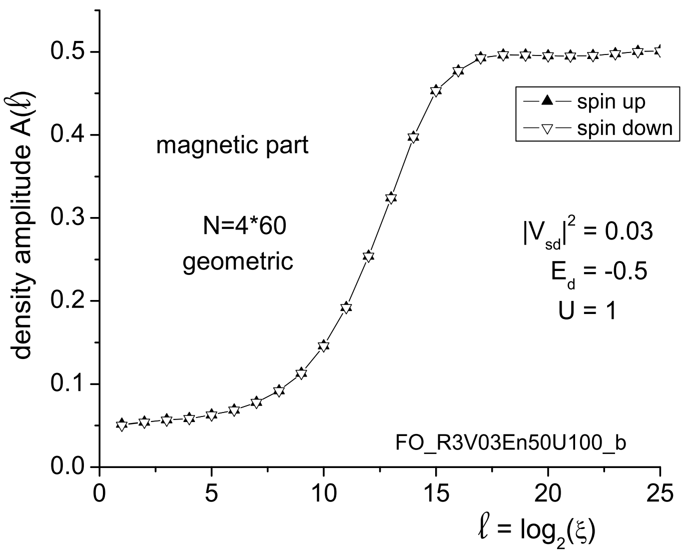

Fig.2: The amplitude $A(\xi)$ of the charge oscillations of the spin-up (full triangle up) and the spin-down (open triangle down) electrons in the magnetic component of the singlet state.

The reason for this apparent contradiction lies in the phase of the different oscillations. The position of the maxima of the charge oscillations may be at ξ_{ma}. In the absence of a phase shift the maxima of the Friedel oscillations would be at integer values of ξ. Therefore the deviation of the ξ_{ma} from an integer, $\delta\xi$, yields the phase shift in units of 2π. The positions of $\delta\xi$of the maxima and minima of the charge oscillations of the spin-up part and the spin-down part of the conduction electrons are plotted in Fig.3. The full triangles show $\delta\xi_{mi}$ of the minima of the charge oscillations and the open triangles represent the maxima. In addition the up-triangles represent the spin-up electrons and the down-triangles the spin-down electrons.

For large distances the maxima positions for both spin orientations lie at 0.75 and the minima at 0.25. Therefore the charge oscillations add constructively in this region. However for distances which are smaller than $\xi_{1/2}$ the maxima and minima of spin-up and down electrons are shifted by ± 0.25 yielding a relative difference of $\delta\xi = 0.5$, corresponding to a phase difference of π. Therefore the charge oscillations of spin-up and down electrons cancel

in this region.

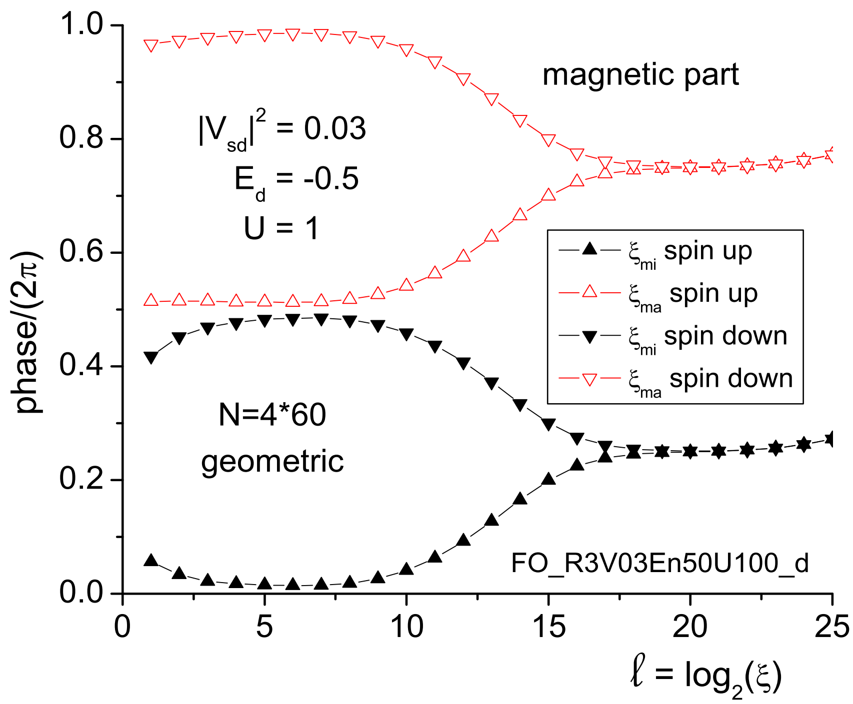

Fig.3: The phase relations of the charge oscillations of the magnetic half of the FA impurity with $U=1, E_d=-0.5$ and $|V_{sd}|^2=0.03$ as a function of the distance $\ell=\log_2(\xi)$. The full and open triangles show the positions (modulo one) of the minima and maxima of the Friedel oscillations for the spin-up and spin-down electron (up and down triangles).

While the total charge oscillation in the magnetic half of the singlet solution cancels essentially to zero in the region of $\ell << \ell_{1/2}$ one obtains a polarization oscillation in this

region. In Fig.4 the amplitude of this polarization in plotted as a function of $\ell = \log_2(\xi)$.

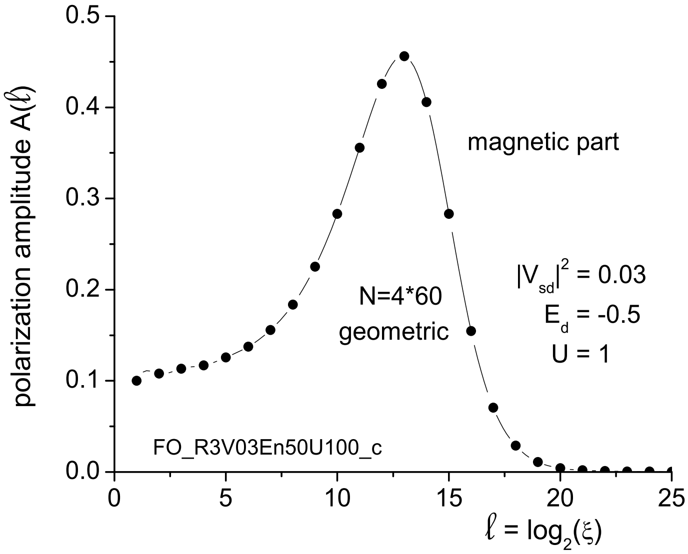

Fig.4: The amplitude of the polarization oscillation of the magnetic magnetic component for the $U = 1$ FA impurity as a function of the distance $\ell = \log_2 \xi$.

If one performs the same analysis for the FA impurity with $U = 0.1, E_d = -0.05$ and $|V_{sd}|^2 = 0.03$ one observes essentially two important differences. Fig.5 shows that (i) the phase difference between spin-up and down electrons at short distances is much less developed than in the local moment example in Fig.3, and (ii) the transitional region where the phases split is shifted to much shorter distances. The fact that the phase differences at short distances is much less than π is the reason that the two charge oscillations of spin-up and down electrons do not cancel. The Friedel oscillations maintain a relatively large amplitude even at short distances.

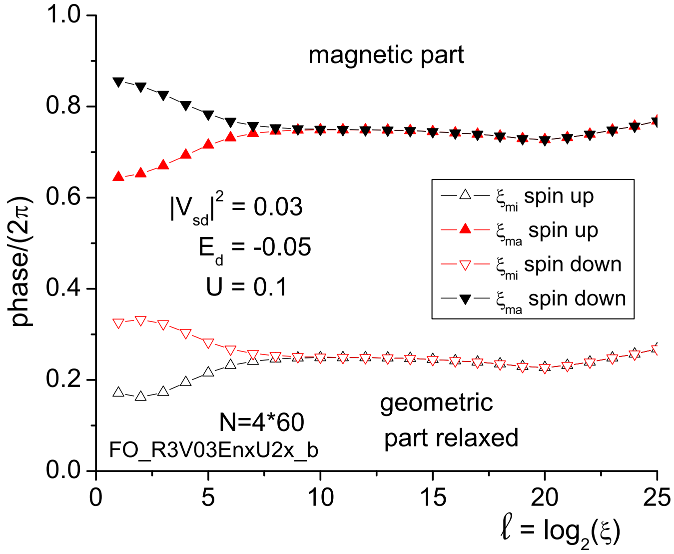

Fig.5: The phase relations of the charge oscillations of the magnetic half of the FA impurity with $U = 0.1, E_d = -0.05$ and $|V_{sd}|^2 = 0.03$ as a function of the distance ξ. The full and open triangles show the positions (modulo one) of the minima and maxima of the Friedel oscillations for the spin-up and spin-down electron (up and down triangles).

3.2 Fermi liquid picture

Nozieres [41] derived from Wilson's renormalization [12] and Anderson's scaling theory [42] a Fermi liquid description of the Kondo effect at low temperatures. In this description, which should also apply to the FA impurity in the local moment regime, the magnetic moment forms a strongly bound singlet state with a conduction electron. This removes the magnetic moment as well as one conduction electron from the system. Virtual excitations cause a weak interacton between the quasi-particles. In ref [32] one of the authors pointed out the similarity between the Friedel oscillations of a Kondo impurity and a Friedel impurity with a very narrow resonance at the Fermi level. This is another confirmation of the Fermi liquid description of a Kondo impurity. In the present paper we want to show that this simililarity also extends to the FA impurity.

Fig.6 shows the Friedel oscillations of a simple Friedel impurity with spin-up and down sub-bands. The resonance d-state lies at the Fermi level, i.e. $E_d = 0$. The s-d-hopping matrix element $|V_{sd}|^2$ is varied by four orders of magnitude between 10^{-1} and 10^{-5}.

There is a remarkable similarity between the Friedel oscillations of the FA impurity in Fig.1 and of the Friedel impurity in Fig.6. If we consider first the Friedel impurity with $|V_{sd}|^2 = 10^{-5}$ then the overall shape of the $A(\ell)$ curve is very similar to the $A(\ell)$-curve for

the FA impurity with $U = 1$. Both curves approach the value two at large distances and zero at short distances. For the Friedel impurity an increase in $\left|V_{sd}\right|^2$ by a factor of 10 shifts the curve by $\log_2(10)$ to the left. The two left curves in Fig.6 no longer reach the value zero. This must be due to the fact that Γ is no longer sufficiently small compared to the band width of one.

We observed a similar behavior for the FA impurity when we reduced the value of U. The similarity with the Friedel impurity suggests that the reason here is also due to the finite band width and not due to the fact that the FA impurity with $U/(\pi\Gamma) < 3$ is no longer in the local moment limit.

For the Friedel impurity with $\left|V_{sd}\right|^2 = 10^{-5}$ the position of the $\ell_{1/2}$ point is at $\ell_{1/2} \approx 12.6$, corresponding to a length of $\xi_{1/2} = 2^{12.6} \approx 6208$. The product between $\xi_{1/2}$ and the resonance half-width $\Gamma = \pi\left|V_{sd}\right|^2 \frac{1}{2} = 1.57 \times 10^{-5}$ is $\xi_{1/2}\Gamma \approx 1.57 \times 10^{-5} * 2^{12.6} \approx 0.10$ (Γ is measured in units of the Fermi energy E_F and ξ in units of half the Fermi wave length $\lambda_F/2$). This product is universal (as long as Γ is sufficiently small compared with band width of the system).

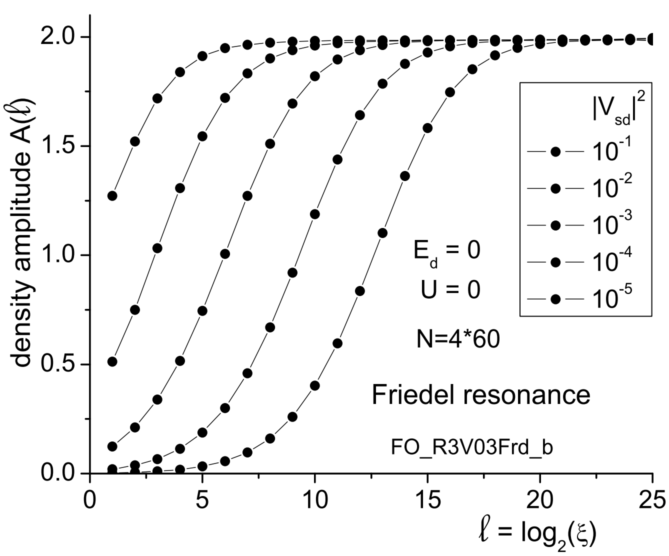

Fig.6: The amplitudes of the Friedel oscillations for different Friedel resonances with $E_d = 0$ and $\left|V_{sd}\right|^2 = 10^{-j}$ with $j = 1, 2, 3, 4, 5$.

We want to quantify this similarity. For this purpose we determine for each curve in Fig.1 and Fig.6 the distance $\ell_{1/2} = \log_2\left(\xi_{1/2}\right)$ where the amplitude $A(\ell)$ has half the saturation value $A\left(\ell_{1/2}\right) = 1$. For the Friedel impurity we plot $\log_2 \Gamma$ of the resonance half-width Γ as a function of $\ell_{1/2} = \log_2 \xi_{1/2}$. That yields the full points in Fig.7.

The similarity between the Friedel curves in Fig.6 and the FA curves in Fig.1 supports the interpretation that the FA impurity has a resonance at the Fermi energy. However, its

half-width is not well known. We assume that it is proportional to the Kondo energy (which is differently defined in different theoretical approaches). We choose for the FA impurity in Fig.1 the definition of the Kondo energy by means of the susceptibility. The latter we obtain through a linear response calculation [43] yielding E_χ. In Fig.7 we plot the logarithm of this Kondo energy $\log_2(E_\chi)$ versus $\ell_{1/2} = \log_2(\xi_{1/2})$ for each curve in Fig.1 (stars). Both sets of points for the FA and the Friedel impurity (circles and stars) lie on two straight lines with the slope of -1 and are separated by a vertical distance of 1.25 which corresponds to a factor of 2.4. If we assign to the FA impurity a resonance half-width of $\Gamma_{FA} \approx E_\chi/2.4$ then the values for Γ_F and Γ_{FA} fall on the same straight line with the slope of -1.

Our calculations of the Friedel oscillations not only show that there is a Kondo resonance at the Fermi level but also suggest that even for relatively small $U/(\pi\Gamma)$ the quasi-particle behavior is similar to that of a Friedel impurity.

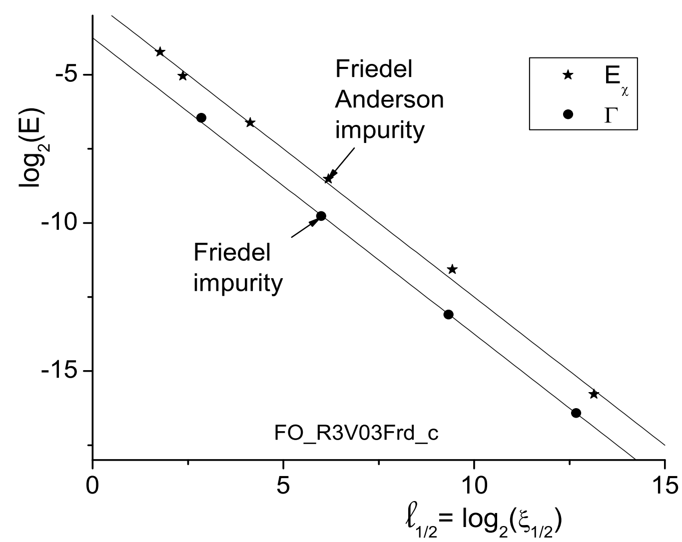

Fig.7: The logarithm of the half-width Γ_F for the Friedel impurity (full circles) and the logarithm of the Kondo energy for the FA impurity are plotted versus the corresponding values $\ell_{1/2} = \log_2(\xi_{1/2})$-values. The latter are obtained from Fig.6 and Fig.1 as the position where $A(\ell)$ takes the value $A(\ell_{1/2}) = 1$. The two full lines are straight lines with the slope minus one. Their vertical separation is 1.25, corresponding to a ratio of $2^{1.25} \approx 2.4$ between Kondo energy and Kondo resonance half width.

4 Conclusion

In this paper we investigate the Friedel oscillations of a set of symmetric Friedel-Anderson impurities. In the local moment limit (large $U/\pi\Gamma$) the normalized amplitude $A(\xi)$ essen-

tially vanishes for short distances and assumes the value 2 for large distances. In this range of $U/(\pi\Gamma)$ the $A(\xi)$-curves show universal behavior because curves for different $U/(\pi\Gamma)$ can be shifted into a perfect overlap. The physics behind this behavior of the amplitude of the Friedel oscillation is illuminated by the study of the simple Friedel impurity with a very narrow resonance at the Fermi level. For these non-interacting Friedel impurities one obtains real space Friedel oscillations which are very similar to those of the interacting FA impurities.

In the case of the Friedel impurity one can derive two conclusions from the Friedel oscillations:

- The amplitude $A(\xi)$ reaches the saturation value of two only when the resonance lies exactly at the Fermi level.
- The $\xi_{1/2}$-point where the normalized amplitude $A\left(\xi_{1/2}\right)$ is equal to one yields the resonance half-width Γ_F through the universal relation $\Gamma_F \xi_{1/2} \approx 0.10$.

The similarity between the Friedel oscillations of the FA and the Friedel impurity supports the concept of a "Kondo" resonance at the Fermi level. The position of the $\xi_{1/2}$-point suggests that the half-width of the FA resonance is of the order of the Kondo energy $\Gamma_{FA} \approx E_\chi/2.4$.

Our calculations of the Friedel oscillations support the concept that there is a Kondo resonance at the Fermi level with the phase shift $\pi/2$ and suggests that even for relatively small values of $U/(\pi\Gamma)$ the quasi-particle behavior is similar to that of a Friedel impurity.

It should be emphasized that the spatial behavior of the FAIR wave function and its charge and spin oscillations provides quantitative information about Kondo energy, Kondo length and resonance width of a FA impurity without the need of a magnetic field or excited states.

References

[1] J. Friedel, Adv. Phys. 3, 446 (1954);Can. J. Phys. 34, 1190 (1956); Nuovo Cimento Suppl. 7, 287 (1958); J. Phys. Radium 19, 573 (1958)

[2] P. W. Anderson, Phys. Rev. 124, 41 (1961)

[3] J. Kondo, Prog. Theor. Phys. 32, 37 (1964)

[4] J. R. Schrieffer and P. A. Wolff, Phys. Rev. 149, 491 (1967)

[5] M. D. Daybell, and W. A. Steyert, Rev. Mod. Phys. 40, 380 (1968)

[6] A. J. Heeger, in Solid State Physics, ed. by F. Seitz, D. Turnbull, and H. Ehrenreich (Academic, New York, 1969), Vol 23, p284

[7] M. B. Maple, in "Magnetism", edited by G. T. Rado and H. Suhl (Academic, New York, 1973), Vol. V, p. 289

[8] P. W. Anderson, Rev. Mod. Phys. 50, 191 (1978)

[9] G. Gruener and A. Zavadowski, Prog. Low Temp. Phys. 7B, 591 (1978)

[10] P. Coleman, J. Magn. Magn. Mat. 47, 323 (1985)

[11] A. C. Hewson, The Kondo problem to heavy Fermions, Cambridge University Press, 1993

[12] K. G. Wilson, Rev. Mod. Phys. 47, 773 (1975)

[13] P. Nozieres, Ann. Phys. (Paris) 10, 19 (1985)

[14] D. M. Newns and N. Read, Adv. in Phys. 36, 799 (1987)

[15] N. E. Bickers, Rev. Mod. Phys. 59, 845 (1987)

[16] P. B. Wiegmann, in Quantum Theory of Solids, edited by I. M. Lifshitz (MIR Publishers, Moscow, 1982), p. 238

[17] N. Andrei, K. Furuya, and J. H. Lowenstein, Rev. Mod. Phys. 55, 331 (1983)

[18] P. Schlottmann, Phys. Reports 181, 1 (1989)

[19] P. Nozieres, and A. Blandin, J. Physique 41, 193 (1980)

[20] L. Kouwenhoven, and L. Glazman, Phys. World 14, 33 (2001)

[21] H. C. Manoharan, C. P. Lutz and D. M. Eigler, Nature (London) 403, 512 (2000)

[22] J. Paaske, A. Rosch, P. Woelfle, N. Mason, C. M. Marcus, J. Nygard, Nature Physics, 2, 460 (2006)

[23] M. G. Vavilov and L. I. Glazman, Phys. Rev. Lett. 94, 086805 (2005)

[24] I. Affleck, and P. Simon, Phys. Rev. Lett. 86, 2854 (2001)

[25] I. P. Simon and I. Affleck, Phys. Rev. Lett. 89, 206602 (2002)

[26] R. G. Pereira, N. Laflorencie, I. Affleck, and B. I. Halperin, arXiv:cond-mat/0612635 (2007)

[27] L. Borda, Phys. Rev. B 75, 041307(R) (2007)

[28] J. Simonin, arXiv:0708. 3604 (2007)

[29] I. L. Aleiner, P. W. Brouwer and L. I. Glazman, Phys. Rep. 358, 309 (2002)

[30] M. Pustilnik, physica stat. solidi (a) 203 1137 (2006)

[31] I. Affleck, L. Borda, H. Saleur, Phys. Rev. B 77, 180404(R) (2008)

[32] G. Bergmann, Phys. Rev. B 78, 195124 (2008)

[33] G. Bergmann, physics today, 32, 25 (August 1979)

[34] G. Bergmann, Phys. Rev. B 74, 144420 (2006)

[35] G. Bergmann, Phys. Rev. B 73, 092418 (2006)

[36] G. Bergmann and L. Zhang, Phys. Rev. B 76, 064401 (2007)

[37] D. E. Logan, M. P. Eastwood, and M. A. Tusch, J. Phys.: Condens. Matter 10, 2673 (1998)

[38] G. Bergmann, Eur. Phys. J. B 75, 497 (2010)

[39] G. Bergmann, Phys. Rev. B 77, 104401 (2008)

[40] H. R. Krishna-murthy, J. W. Wilkins, and K. G. Wilson, Phys. Rev. B 21, 1003 (1980)

[41] P. Nozieres, J. Low Temp. Phys. 17, 31 (1974)

[42] P. W. Anderson, Comments in Solid State Phys. 5, 73 (1973)

[43] G. Bergmann, and Y. Tao, Eur. Phys. J. B 73, 95 (2010)